Journal of Molecular Structure (Theochem), 255 (1992) 485
Elsevier Science Publishers B.V., Amsterdam

AUTHOR INDEX

Bachrach, S.N., 207
Bader, R.F.W., 145, 173
Bertran, J., 283
Bianchi, R., 409
Brinck, T., 271

Cai, X.-H., 327
Carbonell, E., 283
Chang, C., 145
Cioslowski, J., 9
Cremer, D., 189

Destro, R., 409
Duran, M., 283

Esseffar, M., 393

Feil, D., 221

Gatti, C., 409
Ghermani, N., 241
Glaser, R., 45

Harris, B.L., 45

Irle, S., 435

Khoshtariya, D.E., 131
Kraka, E., 189

Laidig, K.E., 93
Lammertsma, K., 309
Lecomte, C., 241
Lin, H.L., 435
Lledós, A., 283
López, V., 393

Mayer, I., 1
McDouall, J.J.W., 35
Meng, L.-P., 327
Merati, F., 409
Mouhtadi, M.El., 393
Murray, J.S., 271

Niu, J.E., 435

Ozerov, R.P., 335

Pearson, R.G., 261

Pichon-Pesme, V., 241
Politzer, P., 271
Popelier, P.L.A., 145

Ritchie, J.P., 297

Schleyer, P.v.R., 309
Schwarz, W.H.E., 435
Slee, T., 173
Solà, M., 283
Souhassou, M., 241
Sudhakar, P.V., 309
Surján, P.R., 9

Tang, T.-H., 327
Tsirelson, V.G., 335

Yáñez, M., 393
Yang, W., 461

Zheng, S.-J., 327

Journal of Molecular Structure (Theochem), 255 (1992) 487–488
Elsevier Science Publishers B.V., Amsterdam

SUBJECT INDEX

Alcohols
A topological analysis of bond activations in alcohols and fluoroalkanes by protonation in the gas phase, 393
Alkylidenecarbene
Quantum topological study on the structure of chemical bonds in alkylidenecarbene and lithiofluoro-carbenoid, 327

Carbonyl oxygen
Properties of atoms in molecules: protonation at carbonyl oxygen, 173
CH_3Cl
Ab initio study of the effect of external perturbations in the dissociation of CH_3Cl, 283
Chemical deformation
Shapes of independent atoms and chemical deformation densities of second-row molecules, 435
Chemical hardness
The electronic chemical potential and chemical hardness, 261
Chemical potential
The electronic chemical potential and chemical hardness, 261
Chemical reactions
Description of chemical reactions in terms of the properties of the electron density, 189
Chemical reactivity
Applications of calculated local surface ionization energies to chemical reactivity, 271
Some comments concerning the use of static charge distributions for predicting chemical reactivity, 297
CN
An ab initio study of hydrogen abstraction from propane by the CN radical, 35
Complimentarity
Similarity and complementarity in chemistry, 145

First order density matrix
The LCAO representation of the first order density matrix in non-orthogonal basis sets: a note, 1
First-row hydrides
Degenerate Li–H exchange in first-row hydrides: a charge density analysis, 309
Fluoride ion
The use of the charge density to investigate chemical reactions; the displacement of methyl chloride by the fluoride ion, 93
Fluoroalkanes
A topological analysis of bond activations in alcohols and fluoroalkanes by protonation in the gas phase, 393

"Hypervalent molecules"
An observable-based interpretation of electronic wavefunctions: application to "hypervalent" molecules, 9

Integrated atomic properties
Efficient new methods for the determination of integrated atomic properties via atom specific electron density functions based on subsets of selected localized molecular orbitals and the reduction of the space of the primitives, 45
Ionization energies
Applications of local surface ionization energies to chemical reactivity, 271

L-alanine molecule
Experimental vs. theoretical topological properties of charge density distributions. An application to the L-alanine molecule studied by X-ray diffraction at 23 K, 409
Large molecules
Electron density and the basic variable: a divide-and-conquer approach to the ab initio computation of large molecules, 461
Li–H exchange
Degenerate Li–H exchange in first row hydrides: a charge density analysis, 309
Lithiofluoro-carbenoid
Quantum topological study on the structure of chemical bonds in alkylidenecarbene and lithiofluoro-carbenoid, 327

Methyl chloride
The use of the charge density to investigate chemical reactions; the displacement of methyl chloride by the fluoride ion, 93

Nucleophilic substitution
A simple quantum mechanical elementary act model for S_N2 nucleophilic substitution in aqueous solutions, 131

Organic compounds
The electron density and chemical bonding in organic compounds by X-ray diffraction, 335

Peptides
Experimental electron density and electrostatic properties of peptides by high resolution X-ray diffraction, 241

Phosphirenes
Topological electron density analysis of halogen-substituted phosphirenes, 207

Primitives
Efficient new methods for the determination of integrated atomic properties via atom specific electron density functions based on subsets of selected localized molecular orbitals and the reduction of the space of the primitives, 45

Propane
An ab initio study of hydrogen abstraction from propane by the CN radical, 35

Quantum chemistry
The molecular electron density distribution. Meeting place of X-ray diffraction and quantum chemistry intermediate between theory and experiment, 221

Similarity
Similarity and complementarity in chemistry, 145

Static charge distributions
Some comments concerning the use of static charge distribution for predicting chemical reactivity, 297